Petr Grigorev | Computational Physicist

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Education

Ghent University/Complutense University of Madrid **Ghent/Madrid**
Ph.D. in Engineering Physics *2012–2017*
International Doctoral College in Fusion Science and Engineering (FUSION-DC)

Peter the Great St.Petersburg Polytechnic University **Saint-Petersburg**
Master in Physics, GPA 5.0 out of 5.0 *2010–2012*
Specialization in Nuclear and Elementary Particle Physics

Peter the Great St.Petersburg Polytechnic University **Saint-Petersburg**
Bachelor in Physics, GPA 4.4 out of 5.0 *2006–2010*
Department of Nuclear Physics

Ph.D. thesis

title: *Assessment of retention of plasma components in tungsten under high flux plasma exposure: multi-scale modelling approach*

supervisors: Dr. Dmitry Terentyev, Dr. Christophe Ortiz

date of the defence: 27 April 2017

description: A new physical model of dislocation mediated H retention in tungsten under fusion relevant plasma exposure conditions was proposed. A Rate Theory simulation tool was parametrised on atomistic data and validated by comparison with experimental results available in literature.

Master thesis

title: *Molecular dynamics study of sputtering of Al, Si and SiC surfaces and nanoclusters by monoatomic and nanocluster beams*

supervisor: Dr. Evgeny E. Zhurkin

Experience

Research

Centre Interdisciplinaire de Nanoscience de Marseille/CEA Saclay **Marseilles**
Post-Doctoral researcher *2020–present*
Project title: *Machine learning in qm/mm simulations of extended defects*
Research tasks:
- Development of a novel hybrid *ab initio*-machine learning method;
- *Ab initio* accurate simulations of dislocation defect interactions;
- Dissemination of the results and search of possible applications of the developed tool set;

Warwick Centre for Predictive Modelling **Coventry**
Research Fellow *2017–2020*
Development and application of a set of atomistic materials modelling methods:
- Hybrid quantum/classical methods to study dislocations and cracks in metals and semiconductors;
- Classical and machine learning based force fields;
- Uncertainty quantification in atomistic models as well as uncertainty propagation in upper scale models;

Belgian Nuclear Research Centre SCK•CEN in collaboration with CIEMAT **Mol/Madrid**
Ph.D. student *2012–2017*

Belgian Nuclear Research Centre SCK•CEN **Mol**
Internship *2012*
Study of radiation hardening of high-Cr steels and model Fe-Cr alloys due to dislocation loops. Results of a large number of MD simulations were analysed in order to provide an input for Dislocation Dynamics (DD) simulation tool.

Petersburg Nuclear Physics Institute **Gatchina**
Bachelor thesis internship *2010*
The internship was done in the laboratory of nuclear and elementary particles physics. During the internship VITESS simulation package was modified and used in order to study the possibility of obtaining monochromatic neutron beams from a fission neutron beam.

Invited presentations

NOMATEN Seminar **NOMATEN Poland**
Hybrid ab initio-machine learning simulations of dislocations *1th February 2023*

Seminar of Service de Recherche en Métallurgie Physique **CEA Paris-Saclay**
Synergistic coupling in ab initio-machine learning simulations of dislocations *7th December 2021*

Seminar of Service de Recherche en Métallurgie Physique **CEA Paris-Saclay**
QM/MM study of hydrogen decorated screw dislocations in tungsten *17th June 2019*

Computational Materials Science Seminar **Skoltech Moscow**
Multiscale QM/MM modelling of materials chemomechanics *10th October 2019*

Awards

Ranked third in the CNRS researchers competition 2023 for section 09

Warwick Faculty of Science, Engineering and Medicine Post-doctoral Research Prize 2020

Service to profession

Reviewer for: Journal of Nuclear Materials, Scripta Materialia, Philosophycal Magazine, Journal of Materials Science and Technology, Computational Materials Science, Nuclear Fusion

Contribution to open-source software: libAtoms/matscipy, Atomic Simulation Environment

Computer skills

Languages: Fortran, C/C++, Python
Operating Systems: Windows, Linux, MacOS
MS Office: Word, PowerPoint, Excel
Simulation packages: LAMMPS, VASP, ASE
SciPy: NumPy, matplotlib, pandas, bokeh
Other: LaTeX, Git, Jupyter notebooks

Languages

Russian: Mother tongue
Italian: A1 CEFR level
English: C1 CEFR level (academic IELTS 7.5)
French: A2 CEFR level (actively learning)